

METHOD FOR SELF-VALIDATION OF MOLECULAR MODELING

ABSTRACT OF THE DISCLOSURE

The present invention provides for a method for validating a computer modeling of a molecular system. The method has the steps of selecting a model parameter of the molecular system; selecting a validation measure of the molecular system; simulating the molecular system by the computer modeling with the selected model parameter; then determining a value of the validation measure of said molecular system from the simulating step; and testing whether the value of the validation measure is in a predetermined range to validate the computer modeling. The method can be performed iteratively by varying the model parameter continuously, such as varying a temperature model parameter, or discretely, such as substituting for different residues in a protein.

15
20
25
30
35
40
45
50
55
60
65
70
75
80
85
90
95
100
105
110
115
120
125
130
135
140
145
150
155
160
165
170
175
180
185
190
195
200
205
210
215
220
225
230
235
240
245
250
255
260
265
270
275
280
285
290
295
300
305
310
315
320
325
330
335
340
345
350
355
360
365
370
375
380
385
390
395
400
405
410
415
420
425
430
435
440
445
450
455
460
465
470
475
480
485
490
495
500